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Determination of the Mott-Hubbard gap in GdTiO3 LARS BJAALIE, Materials Department, University of California Santa Barbara, AMIT VERMA, Department of Electrical Engineering, University of Notre Dame, BURAK HIMMETOGLU, ANDERSON JANOTTI, SANTOSH RAGHAVAN, Materials Department, University of California Santa Barbara, VLADIMIR PROTASENKO, Department of Electrical Engineering, University of Notre Dame, ELIZABETH STEENBERGEN, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, Ohio, DEBDEEP JENA, Department of Electrical Engineering, University of Notre Dame, SUSANNE STEMMER, CHRIS G. VAN DE WALLE, Materials Department, University of California Santa Barbara
— The band gaps of rare-earth titanates are commonly reported to be 0.2-0.7 eV. These values are based on optical reflectivity measurements, from which the onset of optical absorption is derived. Here we report theoretical and experimental results on $GdTiO_3$ (GTO) indicating that the gap is significantly larger. First-principles calculations, based either on density functional theory (DFT) with a hybrid functional or on DFT+U, show that the gap is close to 2 eV. We compare these results with photoluminescence (PL) measurements, which show a strong peak near 1.8 eV, consistent with an observed onset in PL excitation (PLE) at about the same energy. We show that the previously reported optical absorption spectra arise from excitations related to small hole polarons. Given the similarities in electronic structure between the rare-earth titanates, our results for GTO have repercussions for the other members of the series. The results also affect the design of complex-oxide heterostructures involving these materials. This work was supported by ONR and NSF.

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